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Finite Element Simulation Of Laser-Induced Diffusion In Silicon

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Abstract

Laser-assisted diffusion of dopants is a promising way to realize selective emitter solar cells with a reduced number of technological steps. This paper discusses the simulation by finite element method of laser doping in order to optimise the fabrication process. A finite element method is used to solve the heat-transfer equation which describes the thermal effects and Fick’s second law which describes the diffusion of dopants. The phosphosilicate glass (PSG) layer that is produced during the emitter formation on p-type silicon solar cells is used as the doping source during the laser-assisted diffusion process. The influence of laser parameters and material properties are studied. Modelling results are compared to SIMS measurements of the phosphorous doping profile. A structure is discussed in the perspective of a self-aligned process for selective emitter fabrication, where the PSG layer is present underneath the silicon nitride (SiN x) passivation layer.

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1. Introduction

Laser processes are becoming more present in the photovoltaic industry because of the many opportunities they offer. In particular, laser-assisted diffusion of dopants is a promising way to realize at low cost advanced silicon solar cells with high efficiency [1,2]. Along this line, selective emitters, which rely on high dopant concentration localised under the electrical contacts are an effective way to reduce power losses at the front surface of silicon solar cells provided they can be fabricated with a minimum
number of processing steps [3]. The modelling of such laser processes [4] is mostly based on proprietary computer codes. This paper develops a simple model using the finite element software COMSOL® to simulate laser-assisted diffusion in silicon.

2. Experimental

Two test structures are compared to form selective emitters on the front surface of p-type silicon wafers (Fig. 1). In both cases homogenous emitters are formed by thermal diffusion of phosphorous prior to laser processing. In the first structure, the laser doping is performed through the phosphosilicate glass (PSG) directly after the thermal diffusion. In the second structure, the PSG is covered with a silicon nitride (SiN) antireflection coating before laser processing. The simultaneous ablation of the SiN coating and laser-induced dopant diffusion could open the way to a self-aligned selective emitter process with electrochemical metallization. The laser used is a frequency tripled Nd:YAG laser with a wavelength of 355 nm and a pulse duration of 10 ns. The influence of laser parameters is studied to understand the laser-induced doping process.

3. Modelling

Melting, evaporation and dopant diffusion are the main mechanisms that result from the laser-matter interaction. In nanosecond regime, as the optical and thermal penetration depth are much smaller than the diameter of the incident laser beam on the surface, the thermal effects can be described by the heat-transfer equation (1) [5], and the diffusion process can be estimated by solving at the same time Fick’s second law (2). To obtain an estimate of the impact of the laser parameters on the final junction, we use the finite element software COMSOL to solve these two equations.

\[
\rho(T)C_p(T) \frac{\partial T}{\partial t} = \nabla \left[ k_{th}(T) \nabla T \right] + Q
\]  
(1)

\[
\frac{\partial c}{\partial t} = \nabla \left[ D(T) \nabla c \right]
\]  
(2)

\(\rho(T)\) is the material density, \(C_p(T)\) the specific heat capacity, \(T\) the temperature, \(t\) the time, \(k_{th}\) the thermal conductivity, \(Q\) the heat source in volume due to the absorbed laser power, \(c\) the phosphorous concentration in silicon and \(D(T)\) the diffusion coefficient of phosphorous atoms in silicon.

The heat source term \(Q\) in the heat-transfer equation corresponds to the absorbed laser power and can be written as follow:

\[
Q = (1 - R(T))\alpha(T)P_{in}(x,t)I(y)
\]  
(3)
\( \alpha(T) \) is the material absorption coefficient, \( R(T) \) the surface reflectivity, \( P_{in}(x,t) \) the incident laser power and \( I(y) \) the relative intensity given by the Beer-Lambert law. The beam is considered with a Gaussian shape in time and space.

\[
P_{in}(x,t) = P_0 \exp \left\{ -\frac{(t - t_0)^2}{\tau^2} \right\} \exp \left\{ -\frac{x^2}{r^2} \right\}
\]

(4)

\( P_0 \) is the peak power of the laser beam, \( t_0 \) the time shift, \( \tau \) the pulse time, \( r \) the beam radius at half height.

Physical properties of the materials are temperature dependent. We use the smoothed Heaviside function (flc2hs) implemented in COMSOL to describe the abrupt changes with temperatures. Latent fusion heat is taken into account by reducing the heat-source term for the temperatures above fusion by the quantity \( E_{lm} \rho / \tau \). \( E_{lm} \) is the latent fusion heat, \( \rho \) the density and \( \tau \) the pulse duration. The large increase of the phosphorus diffusion coefficient between the solid (\( \approx 10^{-11} \text{ cm}^2 \text{ s}^{-1} \)) and the liquid (4.10^{-4} \text{ cm}^2 \text{ s}^{-1}) phase of silicon allows us to neglect the dopant diffusion below the melting temperature and set it equal to 0. The PSG layer is considered as an infinite source of phosphorus.

In first approximation, texturation of the surface is not taken into account and a plan of symmetry is considered in order to minimize the calculations. The absorption coefficient of Si at 355 nm is around \( 10^8 \text{ m}^{-1} \) and the penetration depth is around 10 nm. Therefore, the minimum element size at the Si surface is 1 nm. To facilitate the meshing, the substrate is divided in different areas in order to have a finer meshing under the irradiated area. The time parameters vary from 0 to 60 ns with a step of 1 ns and 0.1 ns during the laser pulse (from 10 ns to 40 ns).

4. Comparison with experimental results

Phosphorus profiles obtained with the model are compared with experimental data for the first process (Fig. 2a). As expected, simulated curves show the typical behaviour for a laser-assisted diffusion. At higher fluence, phosphorus concentration is more effective, due to a deeper melting of silicon. At the same time the surface concentration decreases.

At high energy (0.5 J.cm\(^{-2}\)), SIMS profiles are well fitted with the simulated curves. At lower energy (0.3 J.cm\(^{-2}\)) experiment and theory present significant differences, which are attributed to the poor pulse-to-pulse repeatability of our laser at this energy level. Indeed, the SIMS measurement averages the
phosphorus concentration over a large area (170 µm diameter). A variability of 30% of the incident laser fluence can cause a significant change in the measured profile (Fig. 2b). Moreover, our simulation results are very similar to those found in the literature [4].

In the case of the second process, simulated phosphorus profiles show similar behaviour. In perspective of self-aligned selective emitters, the laser energy must also be sufficient to ablate the silicon nitride layer. Due to the low absorption coefficient of the silicon nitride, the laser absorption in SiN is negligible and the Si substrate behaves as a heat source after having absorbed the laser energy. The maximum temperature reached in SiN determines the ablation of the antireflection coating. The ablation of the SiN occurs at a temperature around 2150 K. At this point the partial pressure of the N₂ in the SiN reaches one atmosphere and this leads to the dielectric decomposition. Simulation shows that the silicon nitride removal begins with incident laser fluence around 0.35 J.cm⁻² (Fig. 3a), in good agreement with the literature [6] and with our experimental data (Fig. 3b).

5. Conclusion

Finite element calculation software leads to a quick implementation of a model for transient heat transfer and dopant diffusion in silicon. Evolution of the phosphorus profile induced by laser treatment has been computed at various fluences. Theoretical calculation are in very good agreement with experimental SIMS profiles at high laser fluence and point out the critical influence of pulse to pulse laser repeatability at low energy. A self-aligned process for selective emitter fabrication where the PSG doping source is present under the SiNx coating seems compatible with the minimum laser fluence (0.35 J.cm⁻²) required to initiate SiNx ablation and to induced efficient phosphorous diffusion.
Acknowledgements

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References


Appendix: Constants and parameters used

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Name</th>
<th>Value / Fonction</th>
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</thead>
<tbody>
<tr>
<td>Laser fluence</td>
<td>$F_p$</td>
<td>0.5 J.cm$^{-2}$</td>
</tr>
<tr>
<td>Pulse duration</td>
<td>$\tau$</td>
<td>10 ns</td>
</tr>
<tr>
<td>Pulse radius</td>
<td>$r$</td>
<td>12.5 $\mu$m</td>
</tr>
<tr>
<td>Peak power</td>
<td>$P_0$</td>
<td>$2F_p / \sqrt{\tau}$</td>
</tr>
<tr>
<td>Laser wavelength</td>
<td>$\lambda$</td>
<td>355 nm</td>
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<tr>
<td>Absorption coefficient of Si</td>
<td>$\alpha_{Si}$</td>
<td>$10^{-8}$ m$^{-1}$</td>
</tr>
<tr>
<td>Absorption coefficient of SiN</td>
<td>$\alpha_{SiN}$</td>
<td>$10^{-5}$ m$^{-1}$</td>
</tr>
<tr>
<td>Absorption coefficient of PSG</td>
<td>$\alpha_{PSG}$</td>
<td>$10^{-2}$ m$^{-1}$</td>
</tr>
<tr>
<td>Surface reflectance</td>
<td>$R$</td>
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<td>Fusion temperature of Si</td>
<td>$T_{FSi}$</td>
<td>1687 K</td>
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<td>Latent fusion heat of Si</td>
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<td>1797 J.g$^{-1}$</td>
</tr>
<tr>
<td>Heaviside function</td>
<td>$H$</td>
<td>$\text{flc2hs}(T - T_{FSi}, 0.1)$</td>
</tr>
<tr>
<td>Materials properties (ex. density)</td>
<td>$\rho$</td>
<td>$\rho_{\text{SOLID}} + (\rho_{\text{LIQUID}} - \rho_{\text{SOLID}})*H$</td>
</tr>
<tr>
<td>Phosphorus diffusion coefficient</td>
<td>$D$</td>
<td>$H*4.10^4$ cm$^2$.s$^{-1}$</td>
</tr>
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